Typical Product Specifications & Properties

N,N'-Ethylenediamineditetrodotoxin

CAS Number: : 91260-89-8

Specifications	Limits
SMILES	N=1[C@@H]([C@@H]2[C@@H]3[C@@]([C@@H]4[C@@H]([C@@]2([C@@H]([C@@](O4)(O3)O)O)NC1N)O)(O)CNCCNC[C@@]1([C@@H]2[C@@H]3[C@@H](N=C(N[C@@]43[C@@H]([C@@](O[C@@H]1[C@@H]4O)(O2)O)O)N)O)O)O
InChI	LUEUEDMKQXQXQD-UHFFFAOYSA-N
InChIKey	1S/C24H38N8O14/c25-17-29-13(35)5-9-19(39,11-7(33)21(5,31-17)15(37)23(41,43-9)45-11)3-27-1-2-28-4-20(40)10-6-14(36)30-18(26)32-22(6)8(34)12(20)46-24(42,44-10)16(22)38/h5-16,27-28,33-42H,1-4H2,(H3,25,29,31)(H3,26,30,32)

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